EMMO - European Materials & Modelling Ontology

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GOLDBECK CONSULTING

Southampton, 1.5.2019

The EMMO round table

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Examples/Use of Ontologies

- Database integration
  - Connected data
  - Discover new trends
  - New materials candidates

Takahashi, et al (2018). Redesigning the Materials and Catalysts Database Construction Process Using Ontologies. J Chem Inf Mod 58, 1742.

- Easier Database queries
  - Ontology organises data by domain knowledge: contrast to database which is organised by IT need.
  - Querying can be done by scientist using scripts

SCHOTT *presentation, EMMC Workshop, Vienna 2019*

- Integration of analytical processes and equipment

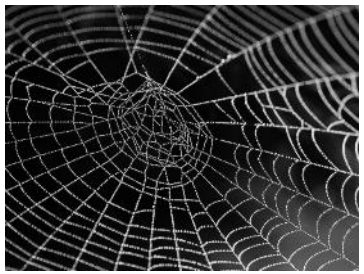
Allotrope Foundation

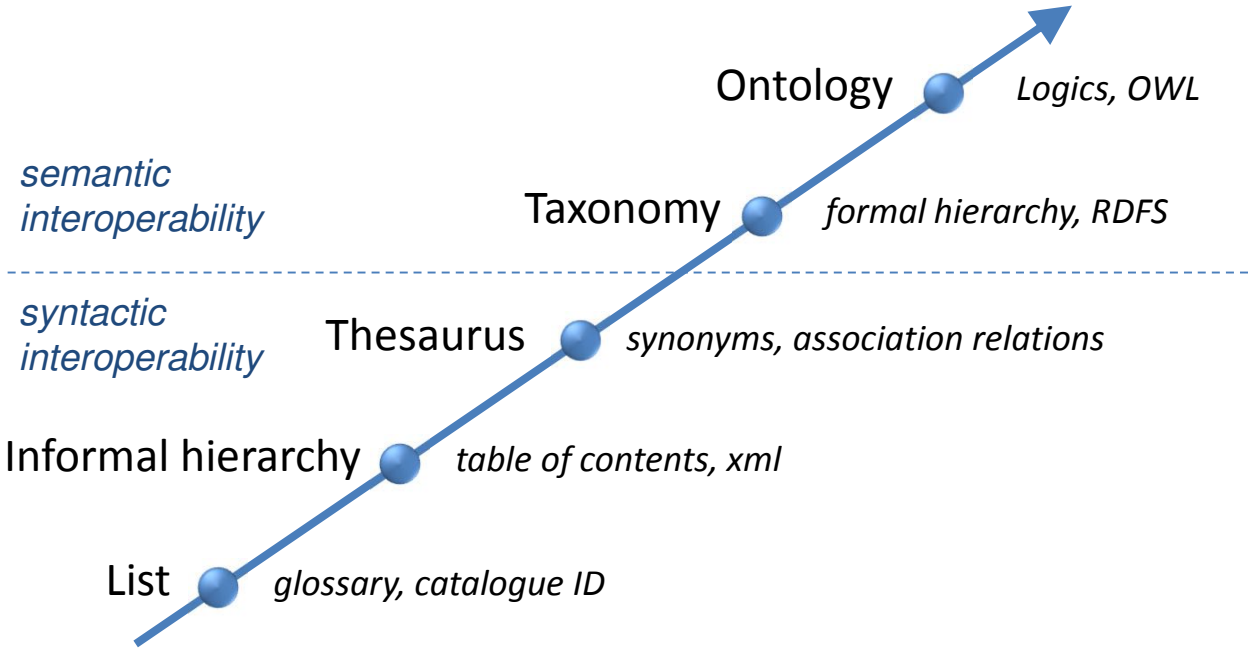
- Integration/collaboration/PLM in complex engineering projects (e.g. ISO 15926 for Oil/Gas industry

POSC Caesar Association

Semantic Spectrum of Knowledge Organization Systems

Semantics and metadata allow a resource to be understood by both humans and machines → promote interoperability.





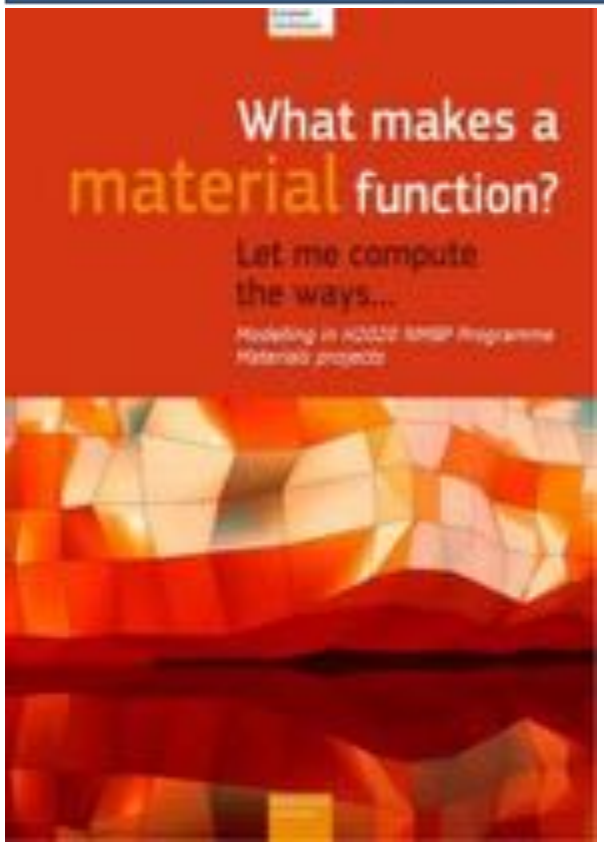
Machine can interpret information and reason.

Machine can process information due to compatible syntax.

Adapted from:
Leo Obrst "The Ontology Spectrum". Book section in of Roberto Poli, Michael Healy, Achilles Kameas "Theory and Applications of Ontology: Computer Applications". Springer Netherlands, 17 Sep 2010.

Speaking the same language

Review of Materials Modelling (RoMM) VII



Definitions of concepts and a harmonised language

Categorizes the models in an interpretable way

Together the physics or chemistry equations and materials relations are called governing equations and they form one model

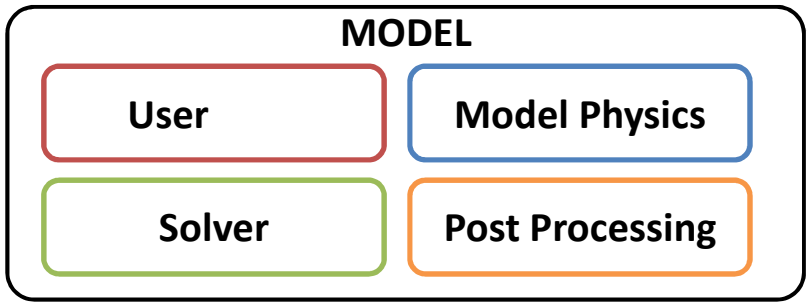
April 2018: The CEN (European Committee for Standardization) Workshop Agreement CWA 17284 “Materials modelling – terminology, classification and metadata”

The “lingua franca” of materials modelling

Modelling-Data (MODA)

MODA for <*user-case*>
***Simulated* in project <acronym>**

OVERVIEW of the SIMULATION			
1	**User Case**	*General description of the User Case.* *Please give the properties and behaviour of the particular material, manufacturing process and/or in-service-behaviour to be simulated. No information on the modelling should appear here. The idea is that this user-case can also be simulated by others with other models and that the results can then be compared.*	
2	**Chain of Models**	**Model 1**	*Please identify the first model. Note these are assumed to be physics-based models unless it is specified differently.* *Most modelling projects consist of a chain of models, (workflow). Here only the Physics Equations should be given and only names appearing in the content list of the Review of Materials Modelling VI should be entered. This review is available on http://cc.europa.eu/research/industrial_technologies/c-library.cfm) All models should be identified as electronic, atomistic, mesoscopic or continuum.*
		Model 2	*Please identify the second model.*
		Data-based model	*If data-based models are used, please specify.*
3	**Publication Peer-Reviewing the data**	*Please give the publication which documents the data of this ONE simulation.* *This article should ensure the quality of this data set (and not only the quality of the models).*	
4	**Access conditions**	*Please list whether the model and/or data are free, commercial or open source. Please list the owner and the name of the software or database (include a web link if available).*	
5	**Workflow and its rationale**	*Please give a textual rationale of why you as a modelier have chosen these models and this workflow, knowing other modeliers would simulate the same end-user case differently.* *This should include the reason why a particular aspect of the user case is to be simulated with a particular model.*	



Finding a common language and formal approach how to log a simulation project

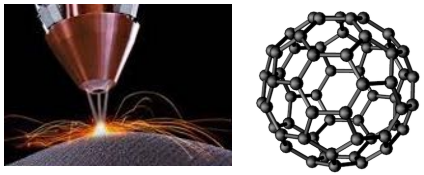
At some point we want a machine to understand it. This is where Ontologies enter!

MODA portal

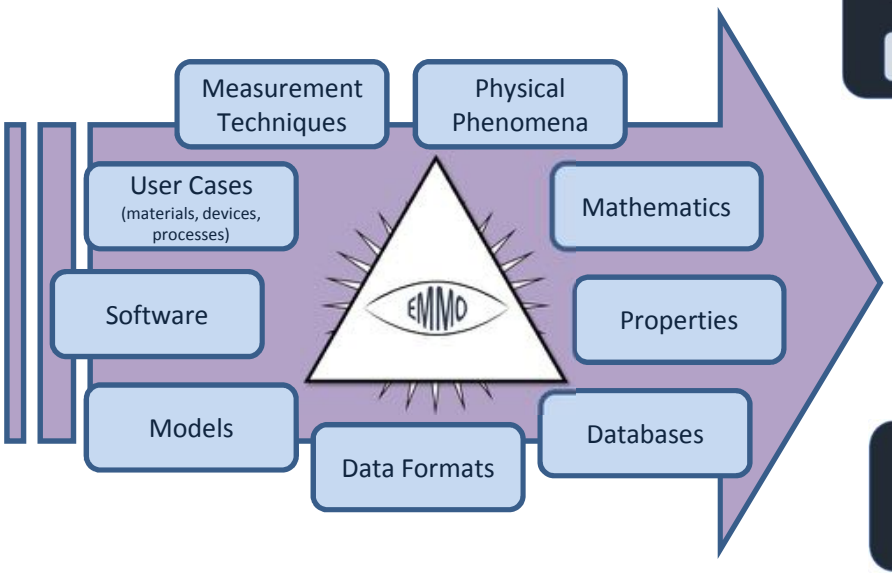
EMMO

Full Name	European Materials & Modelling Ontology
Owners	Emanuele Ghedini (Univ Bologna), Gerhard Goldbeck (Goldbeck Consulting), Adham Hashibon (Fraunhofer IWM), Georg J Schmitz (ACCESS), Jesper Friis (SINTEF)
License	Creative Commons 4.0
Field of Application	Materials (including their characterisation and properties) and Models
Formalisation	OWL-DL
Development Method	Protege, HermiT and FaCT reasoners
Scope	Representation of Physical Sciences including Quantum Mechanics.

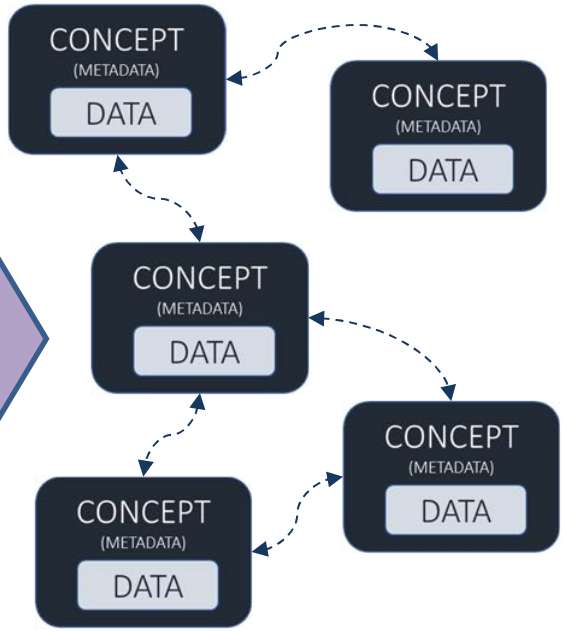
What should EMMO be able to do?



USER CASE
From real world entities…



ONTOLOGY
…built on firm physical science, ICT and analytical philosophy foundations



INFORMATION
…to a digital representation.

EMMO relations

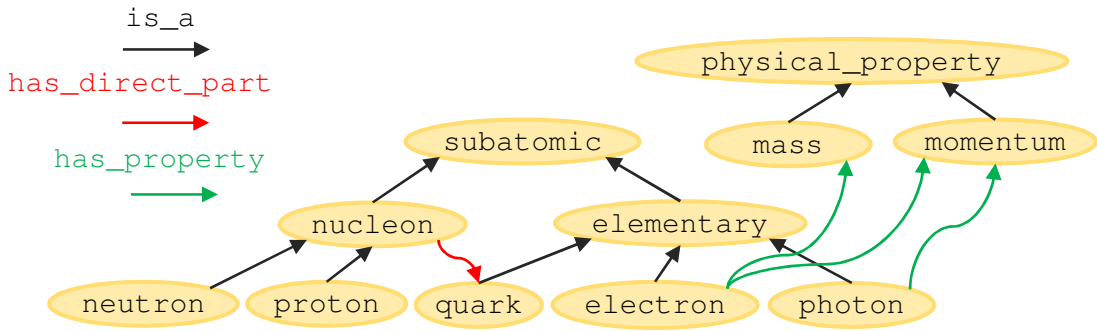
Only 4 primitives

TAXONOMY
Classification
Ex: `is_a`

MEREOTOPOLOGY
Parthood and *Slicing*
Ex: `has_part`

SEMIOTIC
Representation
Ex: `has_property`

SET THEORY
Membership
Ex: `has_member`

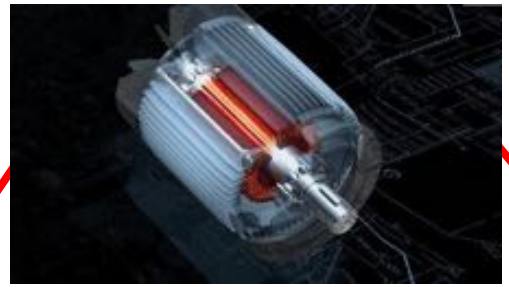


Items that unfolds in space and time
Granularity (multi-scale modelling)

Signs that stands for something else
Represents real-world objects

Abstract collections of items

Peirce Semiotics - Modeller



Representamen/Signifier
Digital Twin

Representation

Interpretation

Matching

Referent/Object
Car Motor

Interpretant/Signifier
Recognises sign

EMMO scope and objectives

EMMO is a formalized system of "signs"

Charles S. Peirce semiotic theory

ONTOLOGY WORLD

SIGN
a physical entity that stands for another physical entity
(an icon, a digital twin, a word, a C++ class)

USER WORLD

INTERPRETER
a human being or a machine that can recognize object attributes
(e.g. color, shape)

INTERPRETANT
the mental/internal representation

PHYSICAL WORLD

OBJECT
any physical entity

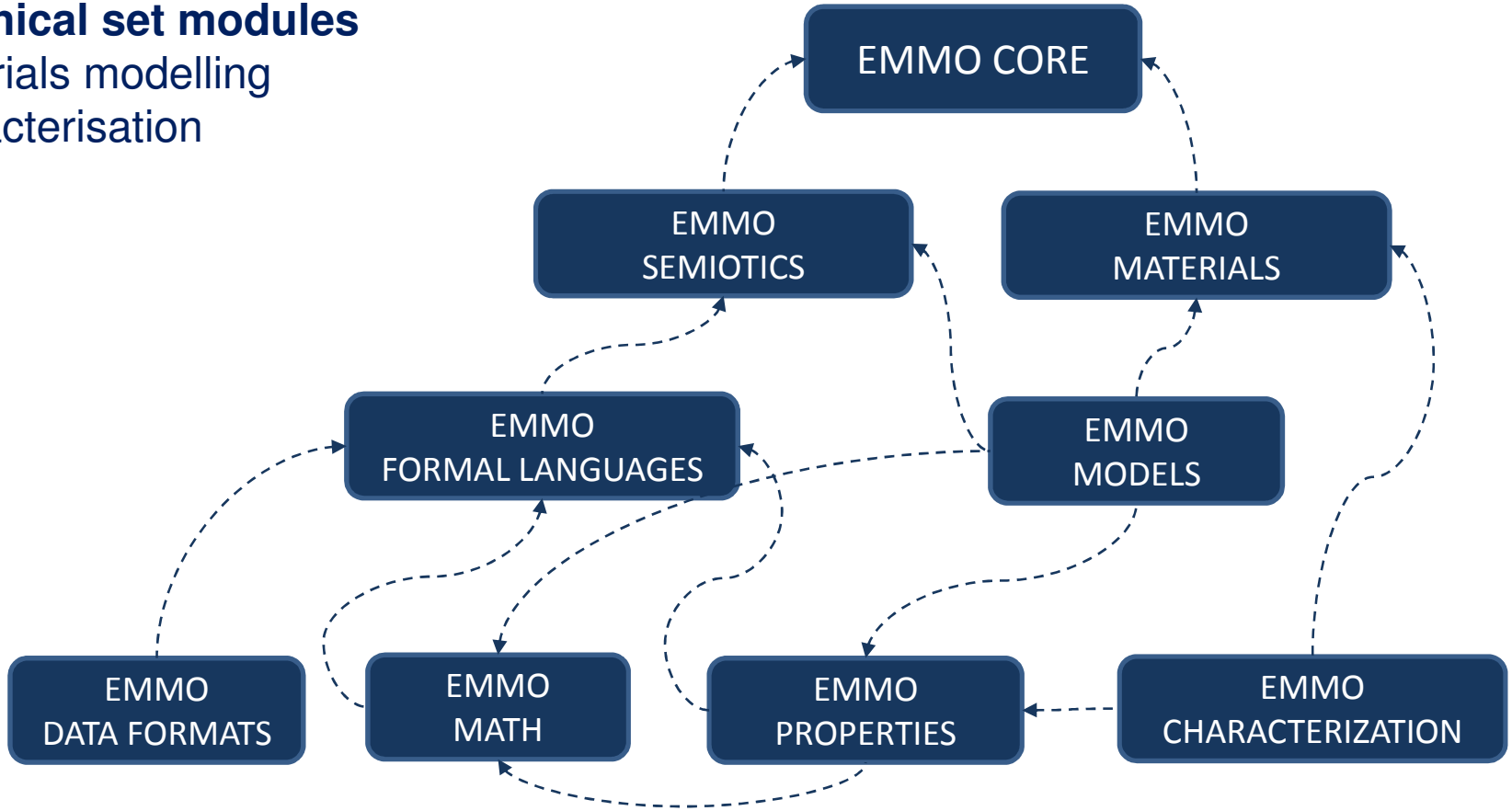
EMMO provides user (interpreter) a way to communicate their interpretations but is not itself an automatic connection between real and ontological world.

EMMO **is not** the truth about the world, only a tool!

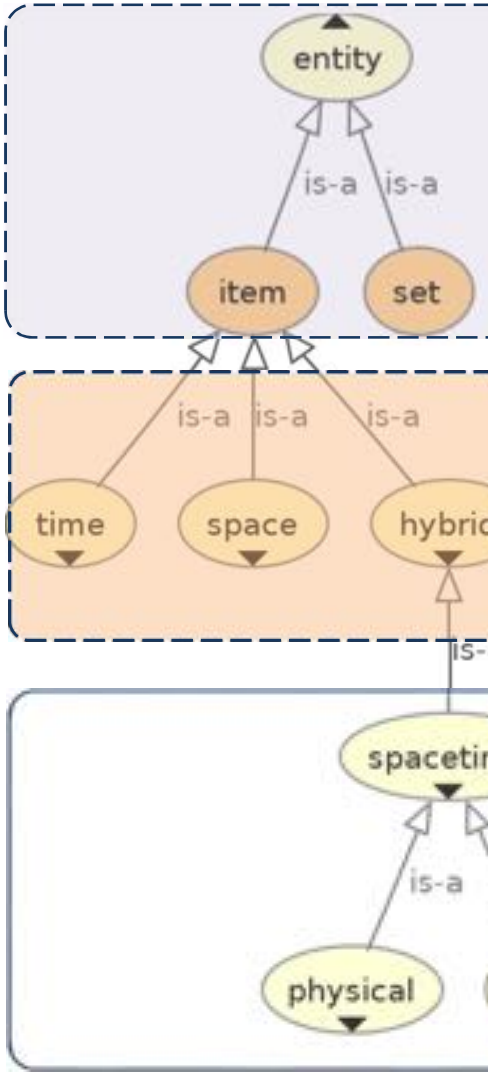
EMMO structure

Hierarchical set modules

- materials modelling
- characterisation



EMMO Core



ABSTRACT CONCEPTUAL LEVEL
Clear separation between **set** (set theory) and **item** (mereotopology).

GEOMETRIC/TOPOLOGICAL LEVEL
items unfold in space (3D) and time (1D) and can be sliced in pure **time**, pure **space** or **hybrid** space and time entities.

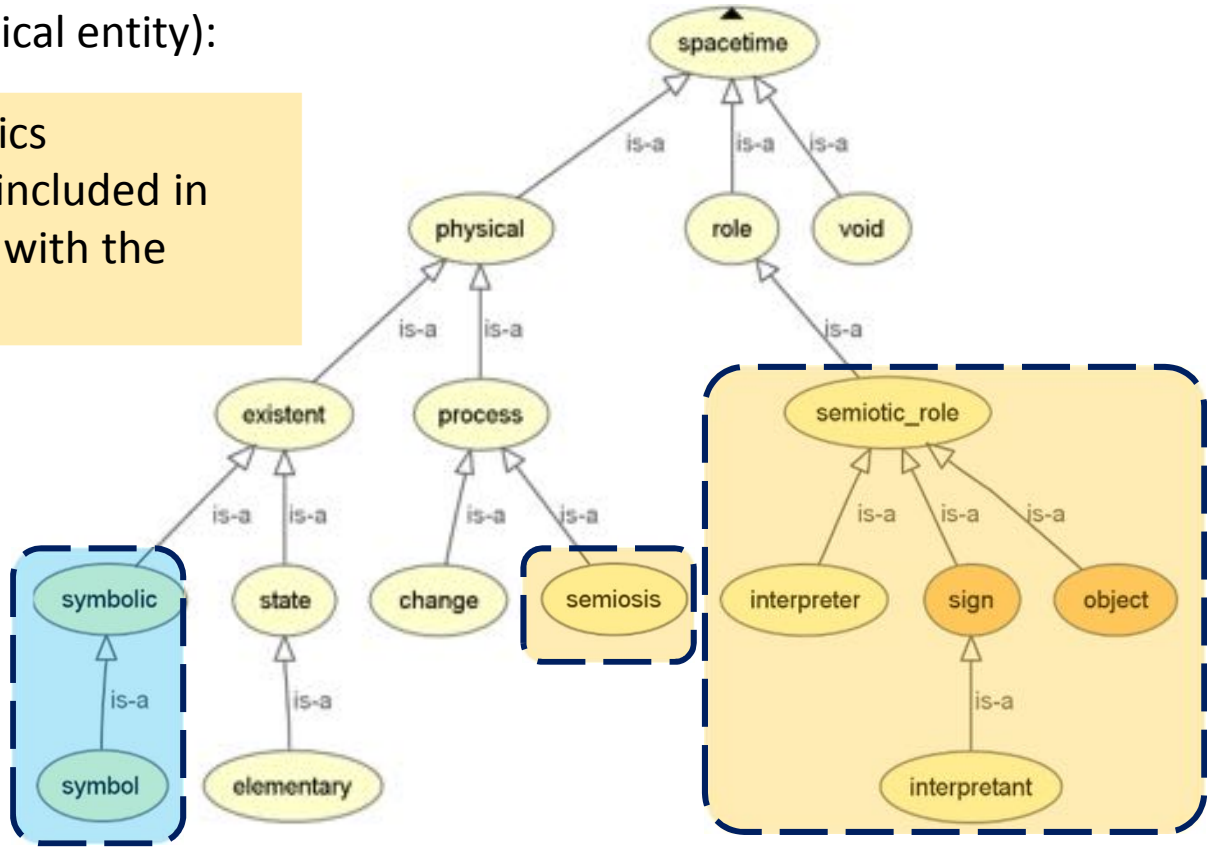
PHYSICAL LEVEL
Real world entities exists only in full 4D **spacetime**
A **spacetime** that can be perceived by (interact with) the interpreter is a **physical**.
If the **spacetime** entity is empty in terms of perception, is a **void**.

EMMO Semiotics

EMMO must represent models and properties (which are signs that stand for a physical entity):

The concepts of Peirce semiotics (**interpreter**, **object**, **sign**) are included in the semiotic branch, together with the **semiosis** process.

Besides that, a branch for representing **symbol**s and **symbolic** entities (e.g. characters, numbers, words) has been introduced, based on formal languages approach.



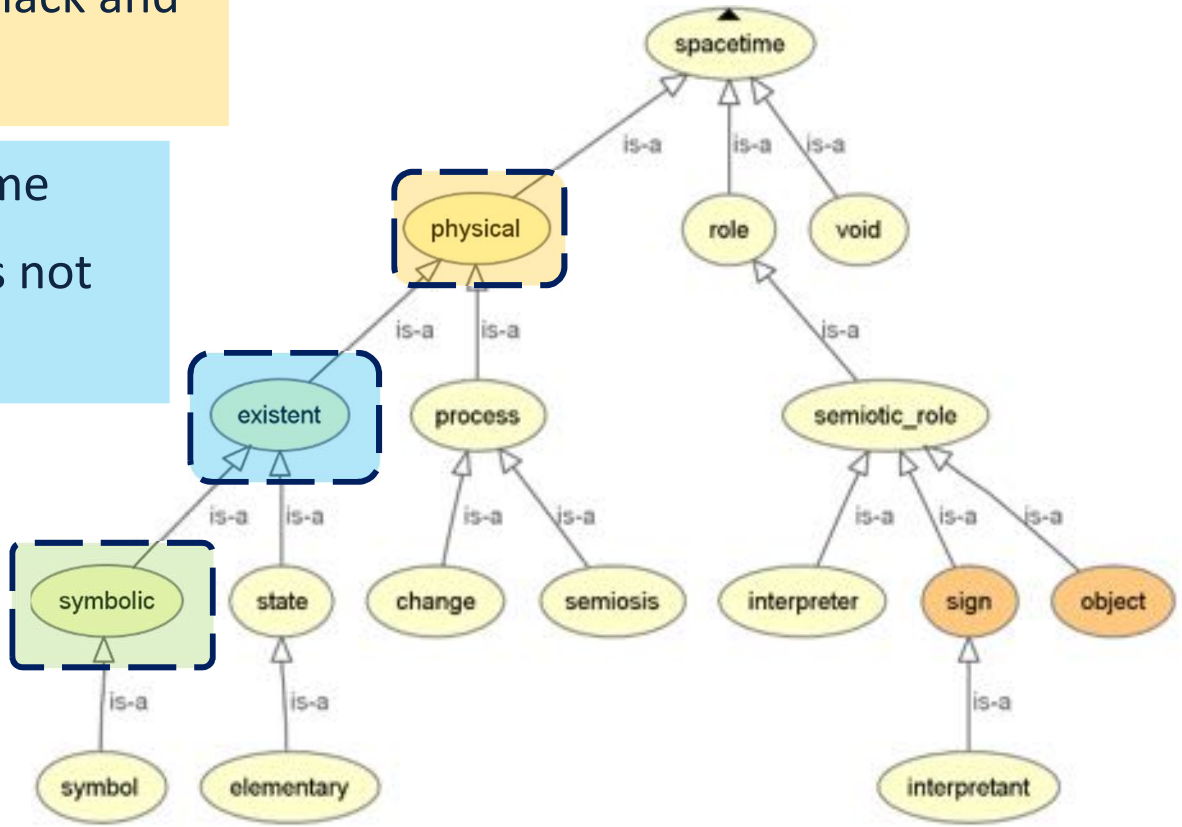
EMMO Semiotics

3.4 kg

it is a physical object, i.e. the black and white pixels on the screen

its a physical that unfolds in time retaining its meaning (i.e. does not change class)

is made of symbols coming from a code (i.e. math and western alphabet) for an interpreter used to this alphabet

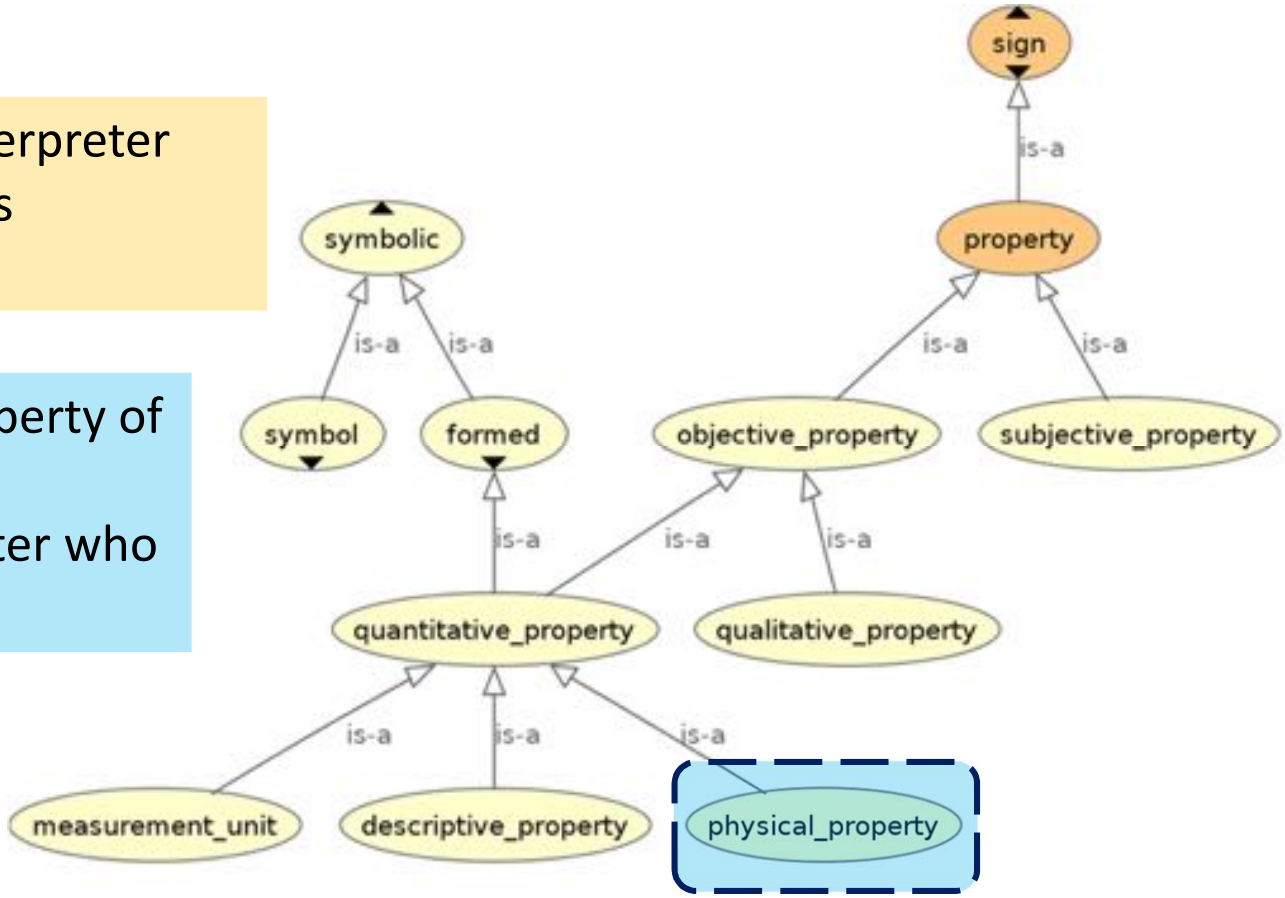


EMMO Properties

3.4 kg

has a meaning for an interpreter who is skilled in numbers measurement units

stands for a physical property of another physical entity according to an interpreter who knows a bit of physics

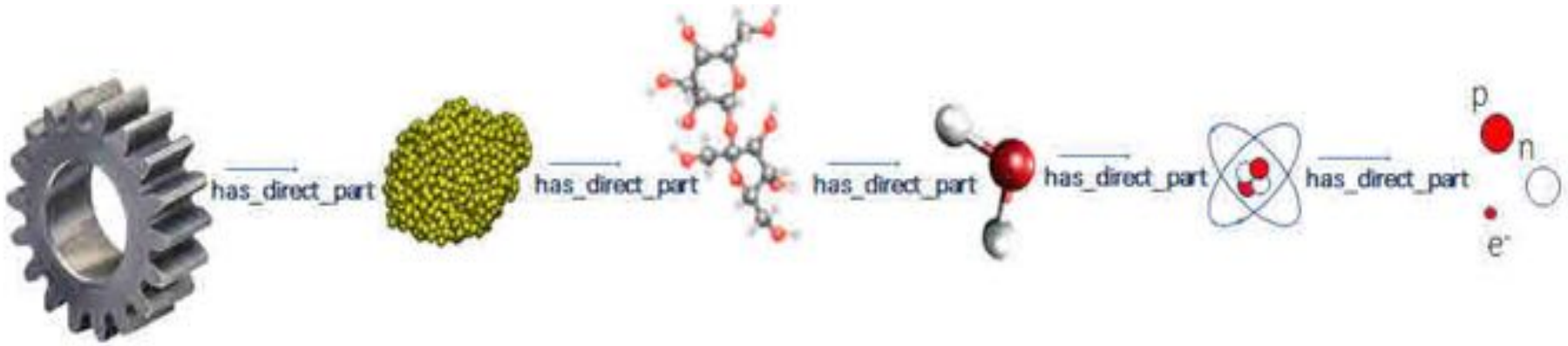


EMMO Materials

EMMO Material Entities are defined by a
Hierarchy of parthood relations,
Including the NEW concept of **direct parthood**

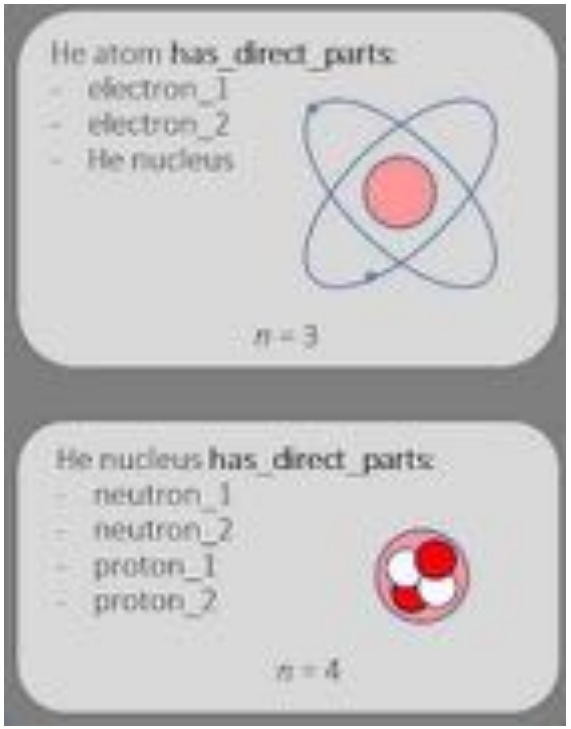
Material can be represented at different levels of granularity.

Hierarchy of structure can be univocally defined.

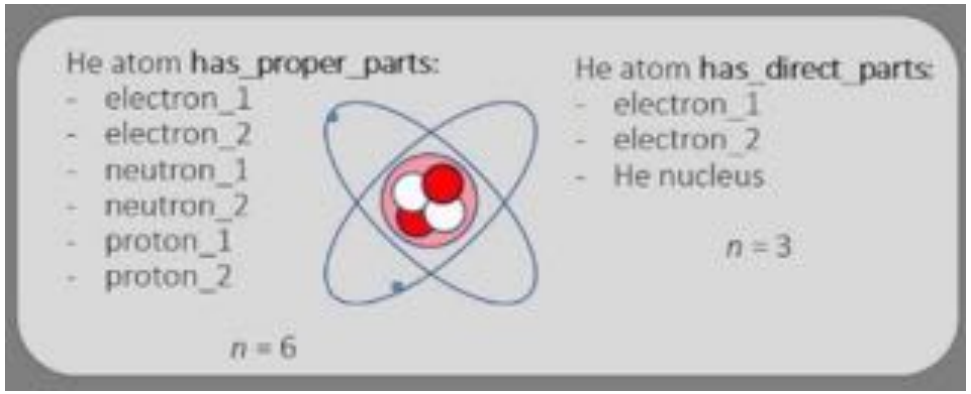


- **Lowest level: Elementary (**the fundamental, non-divisible, constituent of entities)

Axioms, Mereology and Granularity



Has_direct_parts (**Direct Parthood**) gives and retains info about the entities that constitute the direct lower granularity level



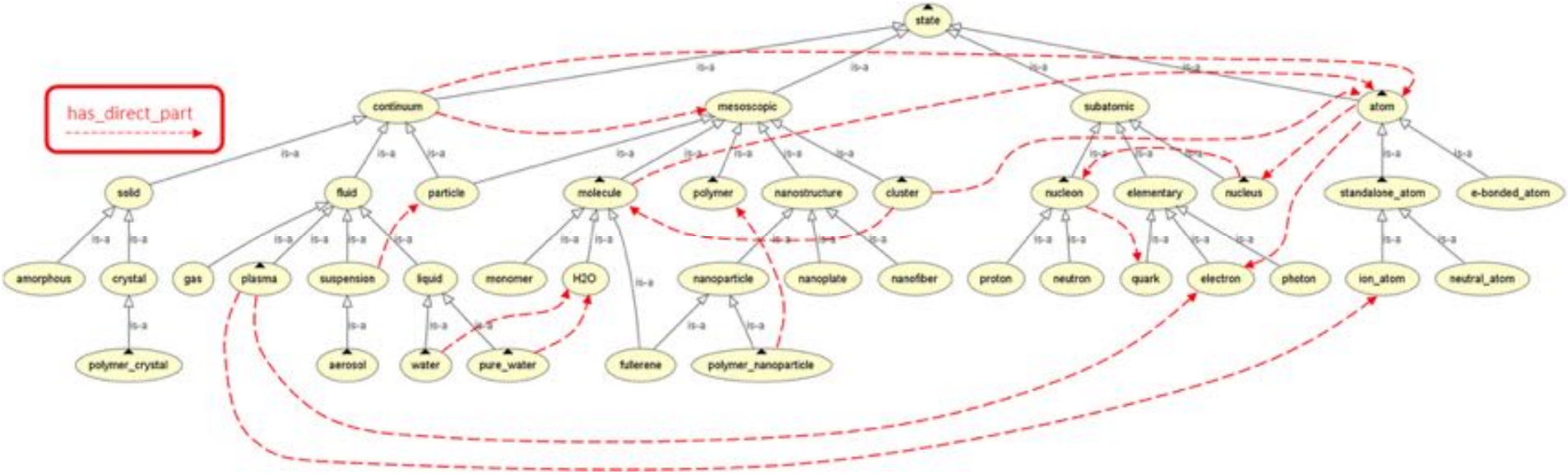
Has_proper_parts (**Proper Parthood**) gives information about all proper parts of an entity at all levels of granularity.

New *Direct Parthood* relation enables a hierarchy of objects with different granularities.

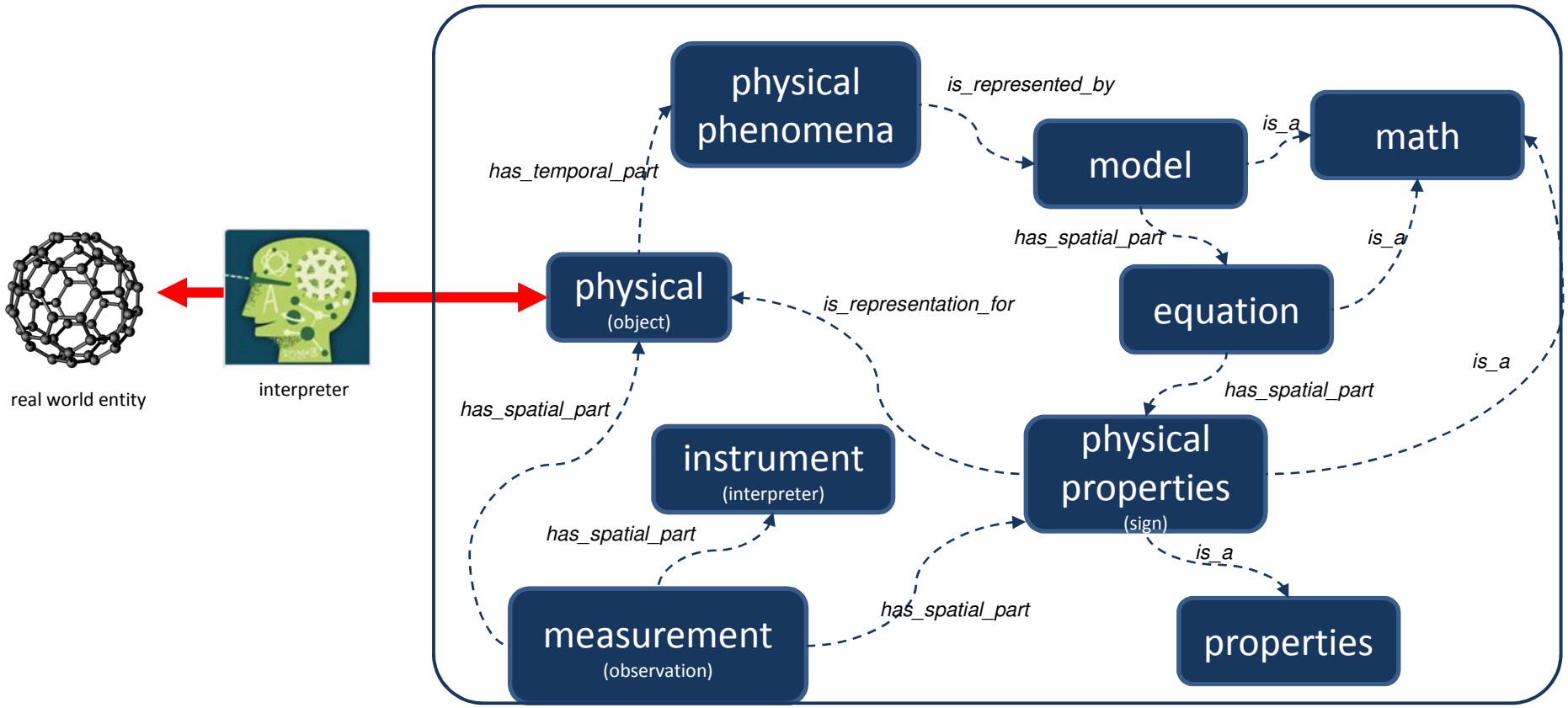
EMMO Material (draft)

Powerful expressiveness of direct parthood in identifying granularity levels.

Strong effect of axioms/logics: e.g. a molecule can't have part crystal

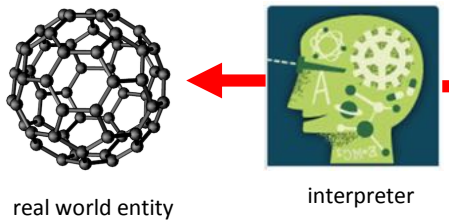


EMMO Properties



EMMO Interoperability

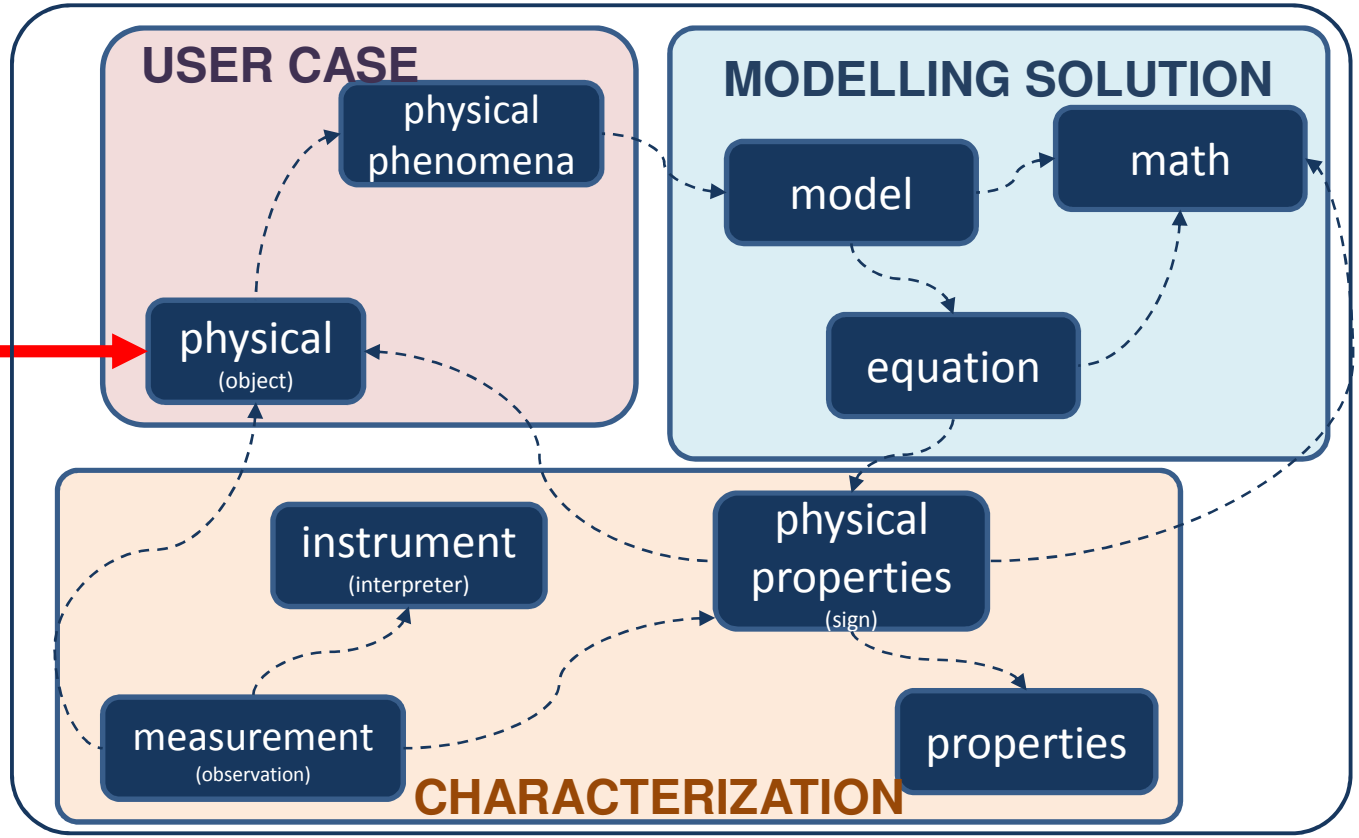
Horizontal interoperability: one user case, multiple modelling solutions.



real world entity

interpreter

Linking between properties database, models and user cases to facilitate **validation** and **data collection**.

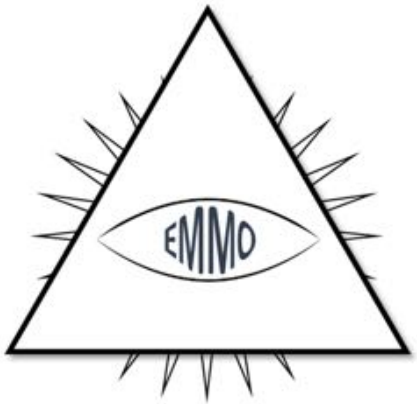


EMMO application fields

Science
standard reference concepts to facilitate understanding across domains

AI and Big Data Analysis
formalized knowledge system ready to be used in AI applications, analytics

Modelling
connections between real world entities and available physical models at different scales



Characterization
Entity-measurement-property connection to facilitate data exchange

Industry
Formalization of the manufacturing process and product, connection with material databases and modelling software

Development and use of EMMO

European Materials Modelling Council - CSA	2019	**EMMO** foundations laid within this CSA project.
Digital Ontology-based Modelling Environment for Simulation of materials	2022	**EMMO** applications cases and integration within a OSP expected within 2020-2021. Team of philosophers, ICT experts and applied scientists.
Materials Modelling Marketplace for Increased Industrial Innovation Virtual Materials Market Place	2022 2021	**EMMO** applied to larger materials modelling communities and marketplaces infrastructures.

… more **existing projects** to involve and more to come in the **next DT-NMBP calls** (hopefully)!!!

EMMC-CSA project has received funding from the European Union's Horizon 2020 research and innovation programme, under Grant Agreement No. 723867.